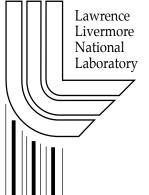
Equivalence Ratio-EGR Control of HCCI Engine Operation and the Potential for Transition to Spark-Ignited Operation

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ABSTRACT

This research investigates a control system for HCCI engines, where equivalence ratio, fraction of EGR and intake pressure are adjusted as needed to obtain satisfactory combustion. HCCI engine operation is analyzed with a detailed chemical kinetics code, HCT (Hydrodynamics, Chemistry and Transport), that has been extensively modified for application to engines. HCT is linked to an optimizer that determines the operating conditions that result in maximum brake thermal efficiency, while meeting the peak cylinder pressure restriction. The results show the values of the operating conditions that yield optimum efficiency as a function of torque and rpm. The engine has high NO_x emissions for high power operation, so the possibility of switching to stoichiometric operation for high torque conditions is considered. Stoichiometric operation would allow the use of a three-way catalyst to reduce NO_x emissions to acceptable levels. Finally, the paper discusses the possibility of transitioning from HCCI operation to SI operation to achieve high power output.

INTRODUCTION

Homogeneous Charge Compression Ignition (HCCI) engines are being considered as a future alternative for diesel engines. HCCI engines have the potential for high efficiency ("diesel-like," [1]), very low nitrogen oxide (NO_x) and very low particulate emissions, and low cost (because no high-pressure injection system is required). Disadvantages of HCCI engines are high hydrocarbon (HC) and carbon monoxide (CO) emissions, high peak pressures, high rates of heat release, reduced speed and stoichiometry range, reduced power per volumetric displacement, and difficulty in starting and controlling the engine.

HCCI was identified as a distinct combustion phenomenon about 20 years ago. Initial papers [2, 3] recognized the basic characteristics of HCCI that have been validated many times since then: HCCI ignition occurs at many points simultaneously, with no flame

propagation. Combustion was described as very smooth, with very low cyclic variation. Noguchi et al. [3] conducted a spectroscopic study of HCCI combustion. Radicals were observed, and they were shown to appear in a specific sequence. In contrast, with spark-ignited (SI) combustion all radicals appear at the same time, spatially distributed through the flame front. These initial HCCI experiments were done in two-stroke engines, with low compression ratio and very high fractions of exhaust gas recirculation (EGR) or trapped (residual) gases.

Najt and Foster [4] were first to run a four-stroke engine in HCCI mode. They also analyzed the process, considering that HCCI is controlled by chemical kinetics, with negligible influence from physical effects (such as turbulence and mixing). Najt and Foster [4] used a simplified chemical kinetics model with encouraging success to predict heat release as a function of pressure, temperature, and species concentration in the cylinder.

Recent analyses of HCCI engines have used detailed chemical kinetics codes [5, 6] in either single zone mode [7, 8], or multi-zone mode [9-11]. Single zone models assume that the combustion chamber is a well-stirred reactor with a uniform temperature, pressure and composition. This model is applicable to homogeneous charge engines, where mixing is not a controlling factor. Single zone analyses can predict start of combustion with good accuracy if the conditions at the beginning of the compression stroke are known, and therefore can be used to explore ranges of operation for different fuels and conditions [12]. On the other hand, single zone models cannot take into account the effect of temperature or concentration gradients that exist inside the cylinder. The assumption of uniform charge temperature inside the cylinder results in all the mass igniting at the same time when the ignition temperature is exceeded. Therefore, a single zone model underpredicts the burn duration, and also overpredicts both peak cylinder pressure and NO_x, and it poorly predicts HC and CO emissions, because HC and CO emissions result from cold mass in crevices and boundary layers, which

are too cold to burn to completion. A multi-zone model [9] can take better account of temperature gradients inside the cylinder, and therefore can do a much better job at predicting peak cylinder pressure, NO_x and burn duration, and generates much improved predictions for HC and CO emissions. These benefits are obtained at the cost of a much-increased time for computation compared with a single zone model. Both models are valuable when judiciously applied.

This paper addresses the problem of controlling combustion in an HCCI engine. This is a challenging problem, due to the extreme sensitivity of HCCI ignition and burn duration to temperature, pressure and composition during the compression stroke. There are many possibilities for HCCI engine control; for example, variable compression ratio, variable valve timing, and operation with multiple fuels. Another possibility has recently been explored by the authors [13]. This possibility is to use a thermal control system. In this thermal control system, thermal energy from EGR and compression work in the supercharger are either recycled or rejected as needed. The thermal control system consists of a preheater to increase fuel-air mixture temperature, a supercharger to increase mixture density and an intercooler to decrease mixture temperature.

Analysis of the thermal control system for HCCl combustion has yielded great insight. The analysis predicts that a thermal control system can be used to successfully control combustion over a wide range of operation, resulting in an engine with higher efficiency than currently achieved by the same engine in diesel mode, while producing very low particulate matter and low NO_x emissions. However, the important analysis of the transient response of the thermal control system is yet to be conducted. The thermal control system includes two heat exchangers (a preheater and an intercooler) to adjust the intake temperature. Use of these heat exchangers may result in slow response to transients under some conditions.

In this paper, the thermal control system proposed in the previous paper [13] is considerably simplified. The preheater, intercooler and supercharger are eliminated, and a throttle plate is added in the intake. The system has three independent control parameters: equivalence ratio, fraction of EGR and intake pressure. These parameters can be tuned to meet the load demands while obtaining autoignition at the desired crank angle and meeting the constraint of maximum pressure. While use of this simplified control system may result in reduced operating range, the simplicity of the system may make it a more desirable choice. In addition to this, the lack of heat exchangers in the system may considerably reduce the response time for the system, making it a more viable choice for vehicular applications.

This paper also discusses the possibility of transitioning from HCCI to spark-ignited operation for achieving higher power output. Being able to operate in SI mode would

likely solve the problem of starting the engine, which is a challenge for pure HCCI engines. Transition between HCCI and SI operation is better accomplished if the HCCI operation range has some overlap with the SI operating range, as has been accomplished in two-stroke engines [14, 15]. For the HCCI range to overlap the SI range, HCCI operation has to be achieved at high equivalence ratio and low EGR, where flame propagation may be fast enough to spread across the chamber in the time available for combustion.

This paper presents engine control maps that show the optimum values of the three free parameters (equivalence ratio, EGR and intake pressure) that achieve the desired output torque and engine speed (rpm). The analysis simulates HCCI engine behavior with a single zone detailed chemical kinetics code (HCT). The engine model is then linked to an optimizer [16] that obtains operating conditions that result in optimum efficiency and performance, while satisfying a peak cylinder pressure constraint. The purpose of this paper is to present a methodology of analysis and optimization that is applicable to real engines. It is recognized that the simplifying assumptions introduced here may not reflect actual conditions in a real engine. However, the results are expected to illustrate the general trends and characteristics that exist for an engine operating in HCCI mode. Furthermore, these "low resolution" results eliminate poor ideas and identify promising strategies that will then be explored using the same methodology, but with a multi-zone combustion model (with an increase in computational time).

ANALYSIS

Figure 1 shows a schematic of the equivalence ratio-EGR control system for an HCCl engine. Combustion in the HCCl engine is analyzed with a single zone HCT model. HCT has been modified to include a simplified analysis of the intake and exhaust processes. The system is analyzed under the following set of assumptions.

- The engine operates at steady-state conditions.
 The problem of transitioning between operating points is not considered.
- Thermal losses in tubes are negligible, e.g., the EGR line is insulated (see Figure 1).
- Exhaust pressure remains at 1 bar.
 Pressurization due to high EGR rates is negligible.
- The combustion efficiency is given by the following expression:

$$\eta_c = 0.94$$
if $\theta_{\text{max}} < 0$ (1)

$$\eta_c = 0.94 - 0.00667\theta_{\text{max}}$$
 if $\theta_{\text{max}} \ge 0$

where η_c is the combustion efficiency and θ_{max} is the crank angle θ for maximum heat release (θ =0 at TDC, θ >0 after TDC). This ad hoc expression is obtained from the experimental results of Christensen et al. [7].

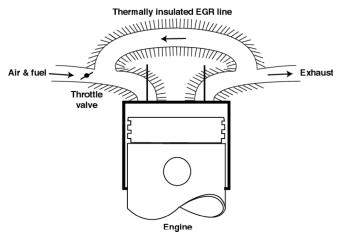


Figure 1. Schematic of the equivalence ratio-EGR control system for an HCCI engine.

The characteristics of the engine and the natural gas fuel used in the analysis are given in Table 1. The dimensions of the engine correspond to the Volkswagen TDI engine, which is well known as a modern diesel engine with high efficiency and performance. The geometric compression ratio (CR) selected for the analysis is CR=12. This was reduced from its original value for the TDI engine (CR=19) to allow for the possibility of transitioning to spark-ignited operation with natural gas.

Table 1. Main characteristics of the Volkswagen TDI 4cylinder engine used for the HCCI experiments and composition of the natural gas fuel.

Engine geometric properties	
Displaced volume	1900 cm ³
Bore	79.5 mm
Stroke	95.5 mm
Connecting rod length	145 mm
Geometric compression ratio	12:1
Natural gas composition, volume %	
Methane	91.1
Ethane	4.7
Propane	1.7
n-Butane	1.4
Nitrogen	0.6
Carbon dioxide	0.5

The engine computations in this study were carried out using HCT (Hydrodynamics, Chemistry and Transport; [5]). HCT has been extensively validated, having been used in a large number of investigations over the years. In particular, HCT was used in studies of engine knock and autoignition [17-19]. The reaction mechanism used in this work includes species through C4 [20], and

models natural gas autoignition chemistry. The mechanism also includes NO_x kinetics [21]. The chemical kinetic reaction mechanisms used by the model for methane ignition and NO_x production have been extremely well established and are widely used. The mechanism includes 179 species and 1125 chemical reactions.

For this paper, HCT is used in single zone mode. As previously discussed, a multi-zone model can yield better predictions for engine performance than a single zone model. However, the much longer running time required for the multi-zone model makes it difficult to make the great number of runs required to generate an engine performance map. The single zone model can predict the conditions necessary for HCCI ignition, and it is therefore appropriate for this application. However, it is necessary to keep in mind that the single zone model overestimates peak cylinder pressure and $NO_{\rm x}$ emissions. Thus, where the single zone model shows peak pressure limits, it is prudent to invest additional time running the multi-zone model.

The computational model treats the combustion chamber as a homogeneous reactor with a variable volume. The mixed temperature of the residual gases and the fresh charge is estimated by a published procedure [22, Chapter 5]. The volume is changed with time using a slider-crank equation [22]. The heat transfer submodel employed in the HCT code simulations uses Woschni's correlation [23]. For simplicity, the cylinder wall, piston and head are all assumed to be at a constant and uniform 430 K, even though this temperature is a function of operating conditions. A thermodynamic model [24] could be used to calculate wall temperatures with accuracy. Exhaust temperature is determined from the temperature of the combustion products at the time of exhaust valve opening (obtained from HCT) and a thermodynamic model for the gas expansion into the exhaust [22]. Engine friction calculations are based on the method by Patton et al. [25]. Patton's model generates an estimate for FMEP, which is then subtracted from the engine IMEP to obtain the engine BMEP.

SYSTEM OPTIMIZATION

For optimization of engine operating conditions, HCT is linked to SuperCode [16]. SuperCode is a gradient-search optimizer originally developed for the U.S. Magnetic Fusion Program for optimizing tokamak reactors and experimental designs [26]. It has subsequently been used to optimize inertial fusion devices, rail-guns, hybrid vehicles [27] and dehumidifiers [28]. SuperCode is well suited for complex optimization problems with multiple decision variables and equality and inequality constraints.

For the engine optimization problem, there are three decision variables that can be adjusted to obtain the desired torque output and rpm, while maintaining

satisfactory combustion and emissions. The three decision variables and their allowable ranges are:

- 1. Fuel-air equivalence ratio, $0.1 \le \phi \le 1.0$
- 2. Mole fraction of EGR, $0.05 \le EGR \le 0.9$
- 3. Intake pressure, 0.1 bar $\leq P \leq 1.0$ bar

A constraint is also introduced in the analysis: The peak cylinder pressure is less than 250 bar. This value is higher than the reported maximum pressure for the VW TDI engine [29]. However, the single zone model used in the analysis is known to overpredict peak cylinder pressure by about 20% [8], so the corresponding peak cylinder pressure for a real engine would be of the order of 200 bar, which is a more acceptable upper limit.

No restriction in NO_x emissions was introduced in this analysis because a NO_x constraint would severely reduce the power output from the HCCI engine. Instead of introducing a NO_x constraint, the possibility is later considered of operating at stoichiometric conditions. Operation at stoichiometric conditions may make it possible to use a three-way catalytic converter for NO_x emissions control.

It is also of importance to set a limitation on the rate of pressure rise, which generally relates to engine noise. Such a constraint is not included in this paper because the single zone model tends to greatly overestimate the rate of pressure rise [9]. A multi-zone model is necessary to obtain reasonable estimates of the rate of pressure rise. It may be possible to find a correlation between the rates of pressure rise predicted by the single zone model and the experimental rates of pressure rise. This would make it possible to use rates of pressure rise obtained from the single zone model as a constraint in the analysis. However, such correlation has not been published in the open literature.

Three different optimizations are done for different operating conditions.

- For any given non-zero torque, the optimizer maximizes the brake thermal efficiency of the system.
- For zero torque (idle), the optimizer finds the conditions for minimum fuel consumption. At idle, efficiency is always zero, so efficiency cannot be used as the figure of merit.
- To determine the maximum torque, the optimizer maximizes torque with no concern for efficiency. However, the peak cylinder pressure restriction still has to be met.

Seventy operating points were selected for generating the performance map. These correspond to ten values of engine speed (600, 1000, 1500, 2000, 2500, 3000, 3500, 4000, 4500 and 5000 rpm) and seven values of torque (0, 10, 20, 30, 40, 50 Nm and maximum torque). The conditions for each of the 70 operating points were obtained by performing an optimization. For each optimization, convergence is achieved after

approximately 60 HCT runs. Considering that each HCT run takes approximately 10 minutes in a 300 MHz Sun Ultra 10 workstation, the total computational time required for generating the performance map is of the order of 700 hours (approximately 1 month). With multizone modeling, the time would extend to several years, unless parallel computing is invoked.

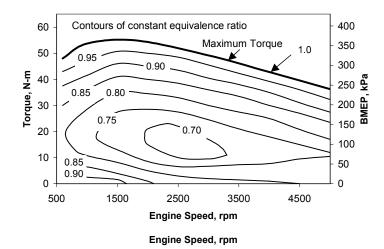


Figure 2. Lines of constant equivalence ratio as a function of torque and engine speed for optimum engine operation as obtained from SUPERCODE. The figure also shows BMEP in the right scale.

RESULTS

Figures 2 through 4 show the optimum values of the three free parameters (o, EGR, P) obtained from SuperCode. Figure 2 shows lines of constant intake equivalence ratio b as a function of torque and engine speed. The figure also shows BMEP in the right scale. The figure shows that the equivalence ratio is minimum in the middle of the speed and torque ranges. The minimum value of equivalence ratio is slightly lower than 0.7. From this point, the equivalence ratio increases as the torque is increased or decreased. The maximum equivalence ratio is reached at the line of maximum torque, where the engine operates with a stoichiometric mixture. Stoichiometric HCCI operation has been demonstrated in a recent experiment [30]. Figure 2 also shows the line of maximum torque (or maximum BMEP) for the engine operating in HCCI mode. The maximum BMEP is only about 3.5 bar. Friction is a significant fraction of the generated power. FMEP varies from slightly less than 1 bar at low speed to almost 2 bar at high speed. To obtain an acceptable power output the engine needs to either be turbocharged or it has to transition to spark-ignited (SI) operation. Transition to SI operation may raise the maximum BMEP to ~10 bar.

Figure 3 shows contours of constant EGR as a function of torque and speed. The figure shows that the mole fraction of EGR is decreased monotonically to increase

the power output. At low power a high fraction of EGR is necessary to obtain satisfactory combustion. At higher power EGR is reduced to increase the amount of fuel inside the cylinder.

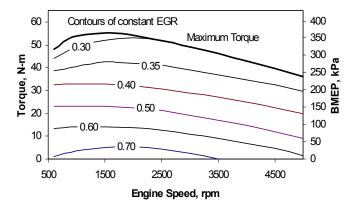


Figure 3. Lines of constant EGR as a function of torque and engine speed for optimum engine operation as obtained from SUPERCODE. The figure also shows BMEP in the right scale.

Figure 4 shows contours of intake pressure. The figure shows that for most of the performance map the engine operates at atmospheric intake, since unthrottled operation results in maximum efficiency. Only at low speed and torque it is necessary to slightly throttle the engine to obtain satisfactory combustion.

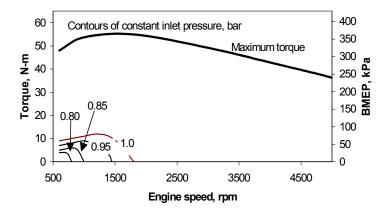


Figure 4. Lines of constant intake pressure as a function of torque and engine speed for optimum engine operation as obtained from SUPERCODE. The figure also shows BMEP in the right scale.

Figure 5 shows lines of constant brake thermal efficiency for the engine operating with the optimum equivalence ratio, EGR and intake pressure shown in Figures 2, 3 and 4. The figure shows that the brake thermal efficiency is quite high for the low power output (BMEP) that is being generated. This is due to the absence of throttling

losses in most of the operating range and due to the fast combustion obtained in HCCI combustion, which approaches the combustion assumed in an ideal Otto cycle.

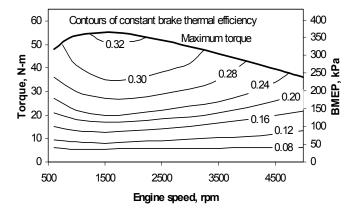


Figure 5. Lines of constant brake thermal efficiency as a function of engine speed and torque for the HCCI engine operating with the optimum equivalence ratio, EGR and intake pressure shown in Figures 2, 3 and 4.

Figure 6 shows lines of constant brake thermal efficiency as a function of torque and rpm for the HCCI engine (repeated from Figure 5). In addition to this, the figure also shows dotted lines, which represent the efficiency of the TDI engine in diesel mode (converted from [29]). The figure shows that the engine working in HCCI mode is more efficient than the engine working in diesel mode. The engine has a higher efficiency in HCCI mode because of the faster combustion obtained with HCCI combustion (approaching the ideal Otto cycle), and the need to delay combustion to reduce NOx emissions in the diesel engine. The diesel engine has some efficiency advantages over the HCCI engine: higher combustion efficiency, and higher compression ratio. However, the HCCI engine still has a higher efficiency for the set of conditions considered here. On the other hand, the maximum torque and power is much higher for the TDI engine in diesel mode (180 N-m).

Figure 7 shows the peak cylinder pressure for the HCCI engine. The figure shows that the peak cylinder pressure is quite low for the low power conditions obtained in HCCI mode, so that the peak cylinder pressure constraint (250 bar maximum pressure) does not play a role in the optimization process. A low compression ratio (12:1) and atmospheric intake contribute to reducing the peak cylinder pressure.

Figure 8 shows lines of constant NO_x in parts per million (ppm) as a function of engine speed and torque. Emission of NO_x is very close to zero for low torque output. The zero NO_x range extends up to 30 N-m at 600 rpm. The region of near zero NO_x includes a good portion of the range of operation in HCCI mode.

However, as the torque is increased from this point, the NO_x increases rapidly, reaching a value of 1000 parts per million at maximum torque. This is a high value of NO_x , which may make it impossible to comply with existing emission regulations. NO_x emissions could be reduced by restricting the range of operation to low values of torque. However, torque output in HCCI mode is already quite low, and it would be highly undesirable to reduce it even further. Please notice that NO_x emissions reported in Figure 8 are calculated with a single zone model that overpredicts NO_x emissions. It would be of great value to compare the predicted NO_x values with results obtained from an experiment or a multi-zone analysis. However, no information is available for this comparison.

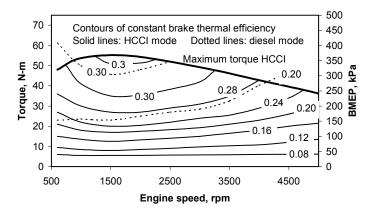


Figure 6. Performance map for the Volkswagen TDI 4-cylinder engine, showing contours of constant brake thermal efficiency. Dotted lines: diesel mode. Solid lines: HCCI mode. A line of maximum torque is also shown for the HCCI mode as a thicker line.

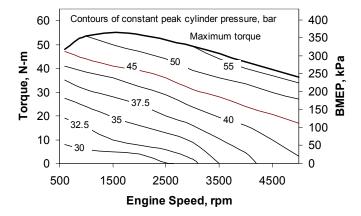


Figure 7. Lines of constant peak cylinder pressure as a function of engine speed and torque for the HCCI engine operating with the optimum equivalence ratio, EGR and intake pressure shown in Figures 2, 3 and 4.

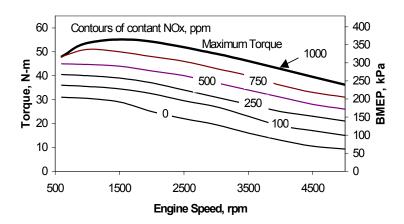


Figure 8. Lines of constant NO_x in parts per million (ppm) as a function of engine speed and torque for the HCCI engine operating with the optimum equivalence ratio, EGR and intake pressure shown in Figures 2, 3 and 4.

STOICHIOMETRIC ENGINE OPERATION FOR NO_x CONTROL

A possibility to achieve lower NO_x emissions without having to reduce the engine maximum torque is to operate the engine at stoichiometric equivalence ratio at the high power conditions where the high NO_x is generated. A three-way catalyst (TWC) could then be used to reduce NO_x emissions. For low torque, the engine can transition to the optimum operating conditions shown in Figures 2, 3 and 4 as the NO_x emissions drop to zero. The potential for using this TWC strategy has been analyzed, and the results are presented in Figures 9 through 11. Figure 9 shows equivalence ratio for the engine operating on stoichiometric mode at high power conditions. The engine operates at stoichiometric for a wide range of conditions in which NO_x is produced. The lower limit of the stoichiometric range was made to coincide with the zero NO_x line presented in Figure 8. This allows the use of a three-way catalyst to reduce the NO_x emissions to levels that may comply with current or future standards. For lower values of torque, Figure 9 shows that the equivalence ratio transitions smoothly to the optimum equivalence ratio shown in Figure 2, so that both figures are identical at the lower part of the figure.

Figure 10 shows contours of constant EGR for the engine operating in stoichiometric mode at high power. The figure shows that EGR for the stoichiometric case is similar to the EGR for maximum system efficiency that was presented in Figure 3. Figures 3 and 9 are identical at the low torque end of the figure, where the engine has transitioned from stoichiometric operation into the optimum operating strategy presented in Figures 2, 3 and 4.

Figure 11 shows contours of constant brake thermal efficiency for the HCCI engine on the stoichiometric operating mode. The figure shows that the efficiency of the engine in stoichiometric mode is slightly lower than the optimum efficiency shown in Figure 5. However, the differences are small. At low power output efficiencies are identical because the engine transitions from stoichiometric operation at high torque to optimum operation at low torque. Stoichiometric operation may therefore be a good methodology to reduce NO_{x} emissions, at the cost of only a small reduction in engine efficiency.

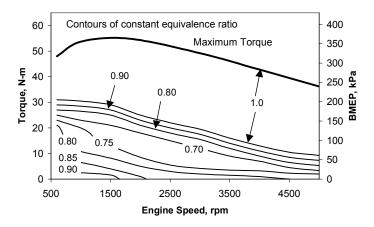


Figure 9. Lines of constant equivalence ratio as a function of torque and engine speed for stoichiometric engine operation at high power for NO_x control. The figure also shows BMEP in the right scale.

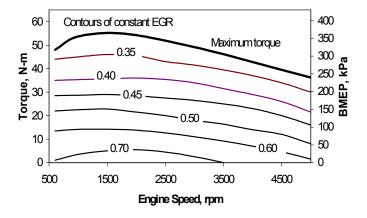


Figure 10. Lines of constant EGR fraction as a function of torque and engine speed for stoichiometric engine operation at high power for NO_x control. The figure also shows BMEP in the right scale.

TRANSITION TO SPARK-IGNITED OPERATION

The HCCI engine analyzed here generates low power output, having a 3.5 bar maximum BMEP. While it is

possible to supercharge the engine to obtain higher power output, it may be simpler to transition to sparkignited mode to obtain high power output (~10 bar BMEP). A hybrid HCCI-SI engine would have the high efficiency at low power that can be obtained with HCCI engines, and the high power output of SI engines. In addition to this, the engine could start in SI mode, solving the startability problem that presents some difficulty for pure HCCI engines.

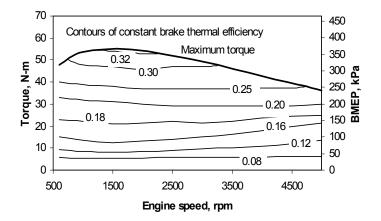


Figure 11. Lines of constant brake thermal efficiency as a function of torque and engine speed for stoichiometric engine operation at high power for NO_x control. The figure also shows BMEP in the right scale.

Transition from HCCI to spark-ignited operation for high power output has been achieved for two-stroke engines by using exhaust throttling [14, 15]. These two-stroke engines present an overlap region where the engine can operate either in spark-ignited mode or in HCCI mode. In the engine being analyzed here, the HCCI engine operates at maximum torque at stoichiometric conditions (ϕ =1) and an EGR fraction of 30% (see Figures 2 and 3). An EGR fraction of 30% approaches the misfire limit in an SI engine [22], thus it is not clear that the engine has an overlap region in which it can operate in both modes. Transition from HCCI to SI mode of operation is a difficult topic that requires further study. A detailed analysis and an experimental verification are necessary to confirm the possibility of transitioning for the conditions analyzed in this paper.

CONCLUSIONS

This work investigates a control system for HCCI engines, where equivalence ratio, fraction of EGR and intake pressure are adjusted as needed to obtain satisfactory combustion. HCCI engine operation is analyzed with a detailed chemical kinetics code, HCT (Hydrodynamics, Chemistry and Transport), that has been extensively modified for application to engines. HCT is linked to an optimizer that determines the operating conditions that result in maximum brake thermal efficiency, while meeting the peak cylinder

pressure restriction. The most important results are summarized next.

- The paper shows operating conditions that result in optimum engine efficiency. Power output did not exceed 3.5 bar. Brake thermal efficiency is high, considering the low power output of the engine. The engine produces high NO_x emissions in the upper range of torque output.
- 2. A strategy is analyzed that reduces NO_x emissions using an exhaust catalyst. The engine is operated at stoichiometric conditions in the region in which the engine produces high NO_x emissions. The possibility then exists of using a three-way catalyst to reduce NO_x emissions. The efficiency of the stoichiometric engine is only slightly lower than the efficiency of the engine at optimum operating conditions, so this may be an acceptable operating condition for low NO_x emissions.
- 3. The paper discusses the possibility of transitioning to spark-ignited operation for achieving high power output. It seems possible that the engine being analyzed could successfully transition from HCCI to SI mode, although a detailed analysis and an experiment is necessary for verifying that transition is indeed possible.

ACKNOWLEDGMENTS

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